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Modelling of hysteresis in two-phase systems

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A MATHEMATICAL FORMULATION for the hysteretic behaviour of a two-phase thermoelastic material undergoing stress-induced coherent martensitic phase transformations is proposed. The hysteresis effects are taken into account by making use of the second principle of thermomechanics and the postulate of realizability. The effective free energy density of the two-phase system is a result of homogenization of the piecewise quadratic potential adopted. The deformation process is formulated as an evolution variational inequality, which is finally solved as a sequence of linear complementarity problems. The answer to the question of existence and uniqueness of a solution to the problem is established. Results of numerical simulations for the shape-memory strips tested under uniaxial tension are included. The strips are initially in an austenitic phase which under prescribed elongation transforms in a martensitic phase and subsequently, after releasing, returns to the initial state. The phase transformation occurs provided its driving force reaches some threshold value, and is accompanied by the energy dissipation and inhomogeneous deformation. The results show the influence of the phase transformation, strain and boundary conditions on the propagation of the transformation front and the deformation mode of the specimen.

1. Introduction

HYSTERESIS IS OBSERVED in many phenomena of physics, engineering mechanics and biology, including ferromagnetism, ferroelectricity and plasticity [20]. In particular, hysteresis effects are induced by the reverse martensitic transformation which is a first-order solid-to-solid phase change occurring in various crystalline solids, e.g. in the pseudoelastic *shape memory alloys*. This special phenomenon is attributed to discontinuous changes in the crystal lattice of the high temperature phase, *austenite*, which possesses a higher symmetry and that of the low temperature phase, *martensite*, which may exist in many variants. The changes in the crystal lattice can be described by homogeneous deformation. The resulting microstructure of shape memory alloys is usually reversible even if they are subject to comparatively large strains.

It is well understood that a phase transformation in crystalline solids is a complex process which takes place in grains at a microscale, [9, 15, 18]. To get an understanding of the process and to tailor the special properties and microstructure of the material, laboratory tests and crystallographic calculations related to this scale are necessary. On the other hand, in order to be able to solve boundary value problems encountered in engineering practice we need possibly simple models which should, however, properly reflect the characteristic features of material behaviour. These are usually phenomenological, macroscopic models of continuum mechanics which are obtained by an averaging procedure. Yet, the fundamental question here is how to find the proper parameters necessary in describing the response of a mixture of phases. On the mathematical side, some averaging procedures corresponding to the relaxation or homogenization of the microscale relations have been studied, in which the notion of a weak solution and the mathematical concepts of Young-measures and H-measures are employed, e.g. [2, 3, 19, 31]. In the field of continuum mechanics, the phenomenological models of phase transformation have been devised in which the microstructural rearrangements are taken into account by means of a set of internal variables with their evolution laws; here we shall cite [40, 13, 30, 11, 12]. The martensitic phase transformation may be induced by temperature or stress. The local self-heating and self-cooling of the material, respectively due to the exothermic character of the austenite-martensite phase transformation and the endothermic character of the reverse one, is the experimentally observed phenomenon [41]. Inclusion of the temperature effects makes the deformation process rate-dependent and highly nonlinear. This is because the stress (more generally, the driving force) of phase transformation depends upon temperature and additionally, the location of the moving heat source (phase front) is not known *a priori*. In this paper we consider the isothermal problem, some numerical results for a nonisothermal one-dimensional case are presented in [10, 8, 43, 23]. So, due to the isothermal assumption our considerations here are related to slow deformation processes in which there is "enough" time for the temperature in the specimen to reach a homogeneous distribution with the value very close to that of the bath.

We propose a mathematically useful description of the hysteretic behaviour which is typically shown by shape memory alloys, extending the approach [24] to a three-dimensional case. It is generally agreed that the appearance of hysteresis in solids undergoing martensitic phase transformations is connected with existence of a nonconvex energy function and some microscopic energetic barriers. The model we use is capable of reproducing the hysteresis, which is mainly induced by frictional effects, through an additional term in the free energy expression, the so-called mixing energy and an extra discrete memory variable. The thermomechanical model applied here was developed by many researchers who contributed to its different aspects and generalizations, MÜLLER *et al.* [16, 33], RANIECKI *et al.* [38, 36, 39, 35, 37], LEVITAS *et al.* [27, 29]. The model is based on quadratic free energies for the parent phase, W_1, and the product phase, W_2. The free energy of the mixture $\widetilde{W}$ (per unit volume) is a weighted sum of the component energies and the "mixing" energy

$$\widetilde{W} = (1 - c)\, W_1 + c\, W_2 + W_{\mathrm{mix}}\,, \tag{1.1}$$

wherein $c \in [0, 1]$ is the volume fraction of the martensitic phase. The final form of (1.1) as given in (2.2) resembles the expression rigorously derived in a mathematical way by KOHN [19] who uses a relaxation procedure at fixed volume fractions, see also PIPKIN [34].

In this paper our aim is to formulate in a unifying manner the corresponding rate boundary value problem for the experimentally observed hysteretic behaviour discussed in [16, 38, 27]. The proposed formulation takes the form of a variational inequality of the first kind, cf. (3.8), which is defined on the product set $U \times K$ where U is the space of kinematically admissible displacements, $\mathbf{u} \in U$, and K is the convex set of admissible volume fractions, $c \in K$. The variational inequality assures the satisfaction in a weak form of both the equilibrium conditions and the phase transformation rules. Furthermore, the domain (in a special case: boundary) between the region where the material is the pure austenite phase and that where it is in the pure martensite state, which is the additional unknown of the problem, is determined automatically as a sort of "by-product" by solving the variational inequality. The rate boundary value problem is integrated in time by an implicit scheme and for its space discretization the finite element method is applied. Finally, the governing variational inequality is solved as a sequence of linear complementarity problems.

2. Free energy and thermomechanical relations

The type of hysteretic behaviour we wish to describe is schematically illustrated in Fig. 1 which corresponds to the experimental results presented in [16], for example. In fact, the stress-strain relations shown were obtained for a one-dimensional bar made of a single crystal CuZnAl alloy, in which the ideal pseudoelastic flow without hardening is a conventional assumption. Our recent results indicate that this hysteretic behaviour is very sensitive to any inhomogeneities, what finally leads to differences between the local response at a material point and the system behaviour [25].

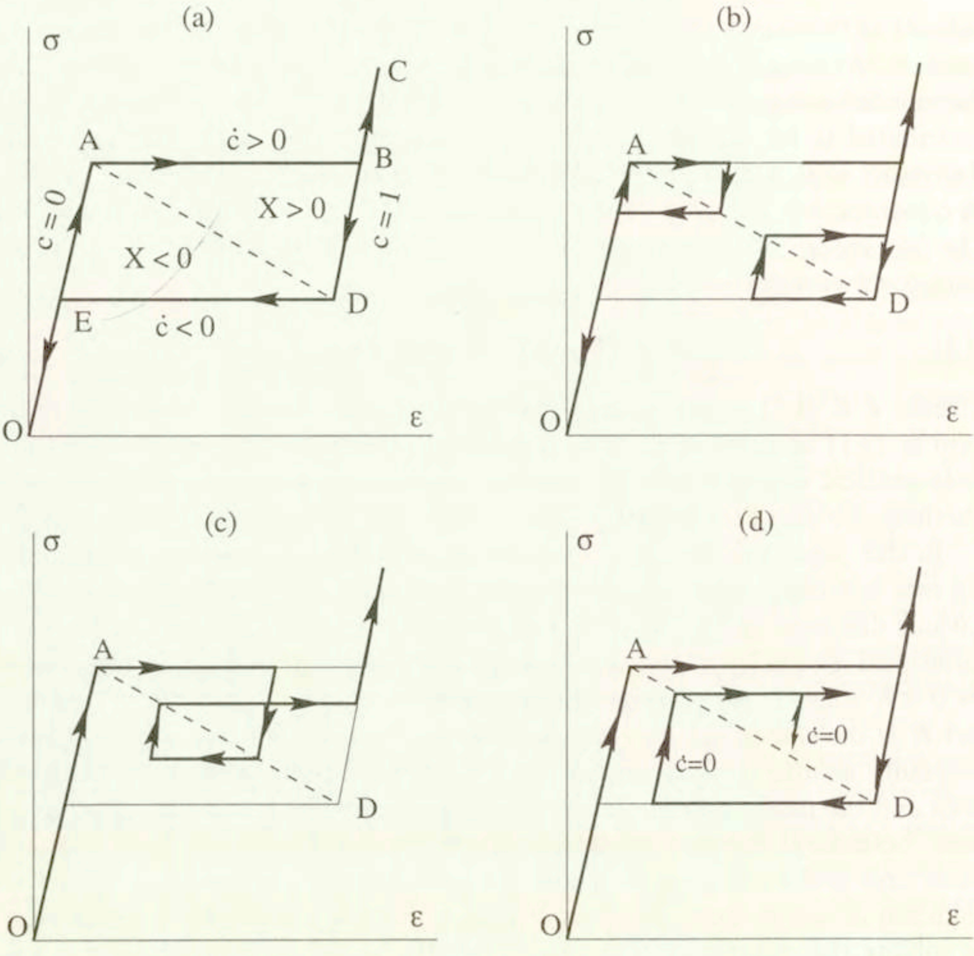


FIG. 1. Stress vs strain diagram of ideal pseudoelastic behaviour. Phase transformation starts at the diagonal AD: (a) Yield and recovery; outer loop. (b) Internal yield and internal recovery. (c) Internal loop. (d) Internal elasticity and history-dependence.

We consider the quasi-static evolution of a two-phase thermoelastic solid which undergoes a martensitic transformation. The problem is treated in the context of small deformations, under the assumption that the material prefers two strain states: the parent phase (austenite), and the product phase (martensite). It may be noted that a two-phase model for martensitic phase transformations is a conceptual simplification as the martensite phase may, in general, appear in many variants, e.g. six variants of martensite in a cubic to orthorombic transformation [4, 5]. We consider the multi-phase problem in [21, 32]. In its natural state at a temperature θ_0 ($\theta_0 > A_f^0$), the body occupies an open region $\Omega \subset \mathbb{R}^d$ with $d = 1, 2, 3$. In a material point (particle) $\mathbf{x} \in \Omega$ we postulate the

Helmholtz free energy W_i, $i = 1, 2$ in the form

$$W_i(\boldsymbol{\epsilon}, \theta) = \frac{1}{2}(\boldsymbol{\epsilon} - \mathbf{d}_i) \cdot \mathbf{E}_i (\boldsymbol{\epsilon} - \mathbf{d}_i) + \varpi_i(\theta),$$

where, for simplicity, the same elasticity tensor $\mathbf{E}_1 = \mathbf{E}_2 = \mathbf{E}$ for each phase is taken. By $\boldsymbol{\epsilon} = \boldsymbol{\epsilon}(\mathbf{u}) = \frac{1}{2}(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}})$ we denote the strain tensor, whereas $\mathbf{d}_i$ is the transformation strain (domain) of ith phase, and a dot $\cdot$ designates the scalar product of tensors. Taking the austenite lattice as the reference state, we may set $\mathbf{d}_1 = \mathbf{0}$ and the transformation strain $\mathbf{d}_2 \equiv \mathbf{d}$. The function $\varpi_i(\theta)$ depends on temperature θ, treated here as a parameter, and we assumed $\varpi_i(\theta) = C_v(\theta - \theta_0) - C_v\theta \ln(\theta/\theta_0) + e_i^0 - \theta s_i^0$ where e_i^0, s_i^0 are the energy and entropy constants of ith phase, C_v the common specific heat. So, the free energy function is a two-well functional which is piecewise quadratic

$$W(\boldsymbol{\epsilon}) = \min\{W_1(\boldsymbol{\epsilon}), W_2(\boldsymbol{\epsilon})\}. \tag{2.1}$$

But, it is known that if the free energy function of the elastic material is not quasiconvex [2, 3, 31], it is possible to find a boundary value problem for which the energy functional has no minimizer. This mathematical property of the phase transformation problem is connected with the "proclivity" of the material to form a finer and finer microstructure, when minimizing the elastic energy. Quasiconvexification of the phase transformation problem is a remedy used for its regularization which leads to an energetically equivalent solution, that is still of great importance. Denoting by c the volume fraction of martensite we can define the free energy of the mixture by

$$\widetilde{W}(\boldsymbol{\epsilon}, c) = \frac{1}{2}(\boldsymbol{\epsilon} - c\mathbf{d}) \cdot \mathbf{E}(\boldsymbol{\epsilon} - c\mathbf{d}) + [(1-c)\varpi_1 + c\varpi_2] + \frac{1}{2}Bc(1-c). \tag{2.2}$$

Observe that the function $\widetilde{W}$ defined in (2.2) corresponds to the relaxation at fixed volume fractions $Q_cW(\boldsymbol{\epsilon})$ derived by KOHN, see Eq. (3.11) in [19]. We recall that for the function W specified in (2.1), its relaxation $Q_cW(\boldsymbol{\epsilon})$ at fixed $c \in [0, 1]$ is defined as, cf. [19],

$$Q_cW(\boldsymbol{\epsilon}) = \inf_{\chi} \inf_{\varphi|_{\partial U} = 0} \frac{1}{|U|} \int_U [(1-\chi)W_1(\boldsymbol{\epsilon} + \mathbf{e}(\boldsymbol{\varphi})) + \chi W_2(\boldsymbol{\epsilon} + \mathbf{e}(\boldsymbol{\varphi}))] \tag{2.3}$$

where $\mathbf{e}(\boldsymbol{\varphi}) = \frac{1}{2}(\nabla\boldsymbol{\varphi} + (\nabla\boldsymbol{\varphi})^{\mathrm{T}})$ and χ, being the characteristic function equal to 0 or 1, describes a partition of U into two phases, with the constraint that the volume fraction of the second phase equals c,

$$\frac{1}{|U|}\int_U \chi = c.$$

By φ we denote the test displacements with vanishing values at the boundary ∂U of U. The minimization in (2.3) is carried out over the physical domain $U \subset \mathbb{R}^d$, with respect to the displacements φ and the partitions of U into distinct phases described by distributions of χ. The set U may be related to the "representative volume element" in the theory of composites. Notice, however, that the austenite-martensite mixture is a special kind of composites in which the volume fractions of constituent phases (variants) are not given *a priori*, but constitute the additional unknowns of the problem. It is not our purpose here to address this aspect in more detail, we only remark that the minimization in (2.3) does not depend upon the domain U. This is a more general result that comes from the theory on quasiconvexification, see [19] for further discussion and references to original sources. In deriving the expression for $Q_c W(\epsilon)$, KOHN [19] has used the relaxation via Fourier analysis with φ being periodic functions. The relaxation of W, denoted by QW, can finally be determined by the minimization of $Q_c W(\epsilon)$ with respect to c over the interval [0, 1]; for a one-dimensional case it is shown schematically in Fig. 2. The most useful property of QW is that it has a minimizer with the corresponding minimal value equal to that of W as defined in (2.1). In this work our point of departure is the function $\widetilde{W}$ by (2.2) which corresponds to Kohn's relaxed energy at fixed volume fractions, $Q_c W(\epsilon)$. We wish to stress the fundamental role which is played here by the term W_{mix}. In the case of the free energy $\widetilde{W}$ of (2.2), W_{mix} depends on the material parameter B, but more general expressions are known in the literature, see [30, 36, 35]. According to [16], the value of B may be related to the area of hysteresis in the elongation-force diagram, another expression for B is given in [19]. In the case $B = 0$, the phase transformation proceeds at a constant stress (the Maxwell line) determined by the "double tangent construction", what in mathematical terms amounts to the convexification of the energy W assigned in (2.1) and is illustrated by the dotted bold line in Fig. 2.

In order to take into account the dissipation and hysteresis which are characteristics of the phase transformation behaviour illustrated in Fig. 1, we minimize the free energy $\widetilde{W}$, defined in (2.2), with respect to c under the requirements imposed by the second principle of thermodynamics, supplemented with the postulate of realizability [28].

From the second law of thermodynamics it follows that the (mechanical) dissipation must be non-negative,

$$\mathcal{D} = \boldsymbol{\sigma}\cdot\dot{\boldsymbol{\epsilon}} - (\dot{\widetilde{W}} + s\dot{\theta}) \geq 0. \tag{2.4}$$

Furthermore, by the standard argument of constrained equilibrium [17, 40], we arrive at the constitutive laws for entropy $s = -\partial\widetilde{W}/\partial\theta$ and stresses $\boldsymbol{\sigma}$,

$$\sigma = \partial\widetilde{W}/\partial\boldsymbol{\epsilon} = \mathbf{E}(\boldsymbol{\epsilon} - c\mathbf{d}), \tag{2.5}$$

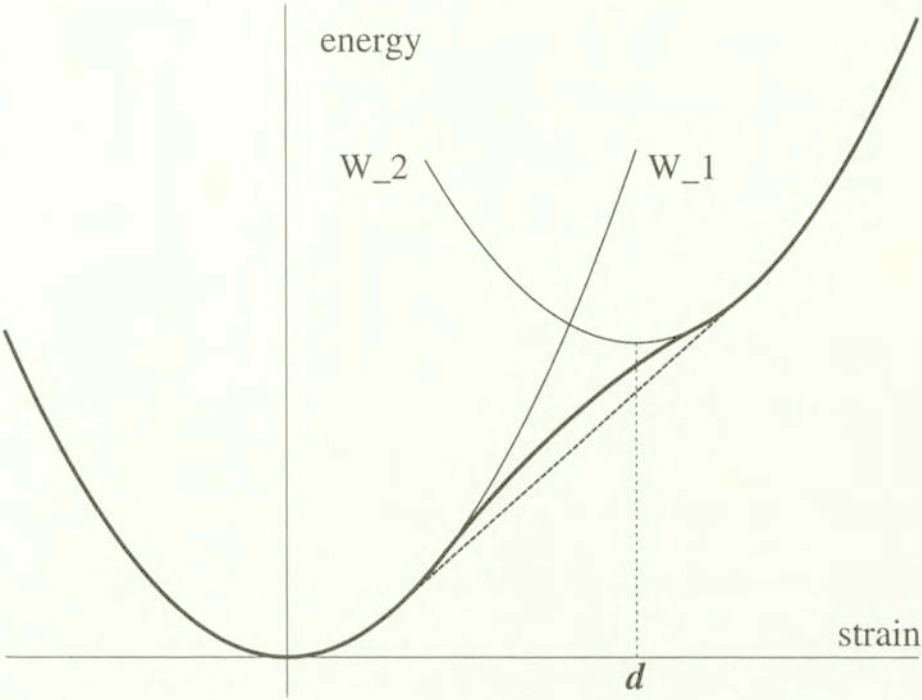


FIG. 2. Quasiconvexified energy function QW for a two-phase system with parabolic energies W_1 and W_2, and transformation strains $\mathbf{d}_1 = \mathbf{0}$, $\mathbf{d}_2 \equiv \mathbf{d}$. The dotted bold line corresponds to the convexification of W.

so that expression (2.4) reduces finally to the inequality

$$\mathcal{D} = X\,\dot{c} \geq 0 \tag{2.6}$$

wherein X is the driving force of phase transformation,

$$X \equiv -\partial\widetilde{W}/\partial c = \boldsymbol{\sigma}\cdot\mathbf{d} - (\varpi_2 - \varpi_1) - \frac{1}{2}B(1 - 2c). \tag{2.7}$$

The condition $X = 0$ defines a plane in the space of stresses $\boldsymbol{\sigma}$, parameterized by the volume fraction c. In the one-dimensional case, $X = 0$ and $c \in [0, 1]$ describe the diagonal AD in Fig. 1. When related to the one-dimensional situation, the driving force $X = X(\boldsymbol{\sigma}, c)$ is positive in the triangle ADB and negative in the triangle ADE of Fig. 1. At this point the following observations can be made.

1. The equilibrium states on the diagonal AD are unstable. Condition (2.6) shows that for $X = 0$ there is no dissipation.

2. As evidenced in Fig. 1, the phase transformation can proceed only if X equals some threshold value and this process possesses some directive tendency which can be controlled by the forward and reverse evolution of c.

Thus, accounting for the dissipation and consequently for hysteresis effects, we assume that phase transformation may take place only if its driving force X reaches some threshold values $\kappa_{1\to2} = \kappa_{1\to2}(c, c^0) > 0$ or $\kappa_{2\to1} = \kappa_{2\to1}(c, c^0) < 0$. The thresholds $\kappa_{1\to2}$ and $\kappa_{2\to1}$ depend upon the current value of volume fraction c and the additional internal variable c^0, which plays the role of a discrete memory. In connection with the type of hysteretic loops shown in Fig. 1, it is reasonable to adopt the following evolution law of the discrete memory c^0 at point $\mathbf{x} \in \bar{\Omega}$,

$$
\begin{aligned}
&\dot{c}^0(\mathbf{x}, t) = 0, && \text{if} \quad X(\mathbf{x}, t) \neq 0,\\
&c^0(\mathbf{x}, t^0) = c(\mathbf{x}, t^0), && \text{if} \quad X(\mathbf{x}, t^0) = 0,
\end{aligned} \tag{2.8}
$$

where t^0 is the time during the process at which the state reaches the diagonal AD in Fig. 1. For the thresholds we have adopted the simple linear expressions

$$
\kappa_{1\to2} = \max\{L(c - c^0), 0\}, \qquad \kappa_{2\to1} = \min\{L(c - c^0), 0\}, \tag{2.9}
$$

in which L is an additional material parameter.

Notice that the functions $\kappa_{1\to2}$ and $\kappa_{2\to1}$ are a measure of the dissipated energy in the course of the forward and the reverse phase transformation, respectively. In fact, relations (2.9) can be derived from the dissipation potential Φ of the form

$$
\Phi(c, c^0) = \frac{1}{2} L (c - c^0)^2, \tag{2.10}
$$

which is a homogeneous quadratic function of the difference $c - c^0$. Expression (2.10) shows that the physical meaning of material parameter $L > 0$ is that of the energy which is dissipated while transforming a unit volume of one phase into the other. We assume that $L \geq B$, whereas the case $L = B > 0$ corresponds to the ideal pseudoelastic flow shown in Fig. 1.

With these understandings, we have the following phase transformation conditions:

$$
\boxed{
\begin{aligned}
&\text{if} && X = \kappa_{1\to2}(c, c^0) && \text{then} \quad \dot{c} \geq 0,\\
&\text{if} && X = \kappa_{2\to1}(c, c^0) && \text{then} \quad \dot{c} \leq 0,\\
&\text{if} && \kappa_{2\to1}(c, c^0) < X < \kappa_{1\to2}(c, c^0) && \text{then} \quad \dot{c} = 0.
\end{aligned}
} \tag{2.11}
$$

It is, perhaps, important to indicate some differences of the hysteretic response pictured in Fig. 1 and a usual phase transformation problem [6]. These are because of the condition $(2.11)_3$, which says that there is no phase transformation for some range of the driving force X, and due to the characteristic internal loops which we model by means of the discrete memory c^0. Clearly, our modelling of the very complex hysteresis loops by means of c^0 should be understood as a first approximation of accounting for internal loops, which is based rather on macroscopic observations. How a memory variable evolves in shape memory alloys under cyclic loading is, however, a difficult and subtle question which requires further research, for related discussions see [42, 1, 7]. In fact, there is no general consensus on the issue what kind of process may proceed from a given state in the upper triangle ABD of Fig. 1d under reloading after unloading: for instance, MÜLLER and his co-workers assert that the reloading is a passive (elastic) process till the previous flow stress, cf. Fig. 5d of [16], but RANIECKI and his co-workers claim that this process is from its beginning an active phase transformation flow, cf. the path ABEH in Fig. 4a of [38]. In this paper we have adopted the simplifying assumption that c^0 is equal to the value of c at the latest state defined by the condition $X = 0$ (the diagonal AD in Fig. 1, for the one-dimensional case). Our discrete memory c^0 may be treated simply as an extra variable which is helpful to follow the internal loops in the diagrams of Fig. 1. However, the use of c^0 is not essential to the approach we develop in this paper. In the particular case we may stipulate that the phase transformation flow will take place only along the interval AB (austenite-martensite phase transformation with $c^0 = 0$) and the interval DE (martensite-austenite phase transformation with $c^0 = 1$). In that case the thresholds assigned in (2.9) become

$$\kappa_{1\to 2} = \kappa_{1\to 2}(c) = Lc, \qquad \kappa_{2\to 1} = \kappa_{2\to 1}(c) = L(c-1). \tag{2.12}$$

Finally we recall the equilibrium equations, which for the stresses defined in (2.5) take the form

$$\operatorname{div}[\mathbf{E}(\boldsymbol{\epsilon}(\mathbf{u}) - c\mathbf{d})] + \mathbf{f} = \mathbf{0}, \tag{2.13}$$

where $\mathbf{f}$ is a body force per unit volume. For the rate boundary value problem considered later on, Eq. (2.13) should be supplemented by appropriate initial and boundary conditions. We assume that the latter are regular, i.e. they satisfy all the relations defining the problem.

3. Mathematical formulation

3.1. Variational inequality

Referring to (2.11) we define the phase transformation functions

$$F_{1\to 2}(\boldsymbol{\sigma}, c, c^0) \equiv \kappa_{1\to 2} - X \geq 0, \qquad F_{2\to 1}(\boldsymbol{\sigma}, c, c^0) \equiv X - \kappa_{2\to 1} \geq 0, \tag{3.1}$$

which correspond to the forward and the reverse phase transformation, and by $\dot{c}^+$ and $\dot{c}^-$ we denote the positive and the negative part of the rate of volume fraction,

$$\dot{c}^{+} \equiv \max\{\dot{c}, 0\}, \qquad \dot{c}^{-} \equiv \max\{-\dot{c}, 0\}, \tag{3.2}$$

so that

$$\dot{c} = \dot{c}^{+} - \dot{c}^{-}.$$

Under these definitions we have the following result, cf. the equivalence lemma in [26].

LEMMA 3.1. *The phase transformation rules (2.11) are equivalent to the rate variational inequality*

$$c \in [0, 1] \qquad F_{1\to2}(c) \cdot (y_{+} - \dot{c}^{+}) + F_{2\to1}(c) \cdot (y_{-} - \dot{c}^{-}) \geq 0 \tag{3.3}$$

$$\text{for all } y_{+},\, y_{-} \geq 0.$$

P r o o f. We prove the assertion in the special case that $c \in (0, 1)$, for the sake of simplicity [1]. First, assume the "if" part of $(2.11)_3$ so that $F_{1\to2} > 0$ and $F_{2\to1} > 0$, then (3.3) implies that $\dot{c}^{+} = \dot{c}^{-} = 0$, because the existence of a $\dot{c}^{+} = p > 0$ would lead to the contradiction: $F_{1\to2}(c) \cdot (y_{+} - p) < 0$ for all $y_{+} < p$. Further, if one of the phase transformation functions is equal to zero, say, $F_{1\to2} = 0$, i.e. the "if" part of $(2.11)_1$, then $\dot{c}^{+} > 0$ satisfies (3.3) (a degenerated case $\dot{c}^{+} = 0$ is also covered). Note that by (3.1), $F_{1\to2} = F_{2\to1} = 0$ is possible only for the states on the diagonal AD in Fig. 1 and if the thresholds are defined as in (2.9); such a coincidence is not possible for thresholds assigned by (2.12). Finally, by satisfying inequality (3.3) on the positive cone $\mathbb{R}_{+}$, with $\dot{c}^{+}, \dot{c}^{-} \in \mathbb{R}_{+}$, we enforce the conditions (3.1). This completes the proof.

Inequality (3.3) implicitly defines the evolution law of c, thereby the kinetics of the strain induced by the phase transformation. Usually, the evolution law for the volume fraction variable is written in the form of an equation for the active phase transformation process which is the pivotal concern in the metallurgical literature. However, from the standpoint of computational mechanics one of the main difficulties lies in the determination of the domain in a body where the forward and reverse phase transformations do take place, i.e. where the evolution law(s) of c with $\dot{c} \neq 0$ is in force, and the domain where the response is elastic and a different constitutive law with $\dot{c} = 0$ holds. The variational inequality encompasses both the "active" and the "passive" evolution of c, playing the role of a switch. It may be remarked that the above formulation of the phase transformation criteria is similar to that of the loading/unloading conditions in the flow theory of plasticity [26]. Yet, one of the main differences is due to the

[1] The case $c = 0$ or $c = 1$ leads to the expression for X, cf. [24], which includes the subdifferential of the indicator function, $\partial I_{[0,1]}(c)$, so that (3.1) will hold for any $c \in [0, 1]$.

constraint $c \in [0,1]$ and that imposed on the plastic multiplier λ which is bounded only from below and whose rate must be non-negative, i.e. $\lambda \geq 0$, with $\dot{\lambda} \geq 0$.

From the computational reasons, it is natural to express the functions (3.1) in terms of displacements through the strain tensor. This leads to the new phase transformation functions

$$
\begin{aligned}
G_{1\to 2}(\boldsymbol{\epsilon}, c, c^0) &\equiv -\mathbf{d}\cdot\mathbf{E}\boldsymbol{\epsilon} + (\mathbf{d}\cdot\mathbf{E}\mathbf{d} - B)\,c + \kappa_{1\to 2}(c, c^0) \\
&\qquad\qquad\qquad\qquad + (\varpi_2 - \varpi_1) + B/2, \\
G_{2\to 1}(\boldsymbol{\epsilon}, c, c^0) &\equiv \mathbf{d}\cdot\mathbf{E}\boldsymbol{\epsilon} - (\mathbf{d}\cdot\mathbf{E}\mathbf{d} - B)\,c - \kappa_{2\to 1}(c, c^0) \\
&\qquad\qquad\qquad\qquad - (\varpi_2 - \varpi_1) - B/2.
\end{aligned}
\tag{3.4}
$$

The formulation discussed above constitutes a natural advantageous basis for the numerical treatment of the problem. Toward this end, the finite-dimensional counterpart of the variational inequality (3.3) in terms of the phase transformation functions (3.4) is obtained by the finite element method, and its evolution in time is solved as a sequence of linear complementarity problems.

3.2. Incremental problem

For boundary value problems of practical significance it is necessary to solve the evolution problem (3.3) in a weak form with respect to the space variable, and incrementally in time. To this end, the relations (3.4) will be expressed in displacements through the strain tensor and imposed to be valid for the body Ω as a whole. Doing this, from (2.6) we arrive at a reduced form of the global Clausius-Duhem inequality [14]. Problem (3.3) is a free boundary problem in which the boundary between the pure phase region in which $c = 0$ or $c = 1$ and the phase transformation region in which $c \in (0,1)$ is not known in advance. Furthermore, the hysteresis loops depend also on the discrete memory variable c^0. Due to this kind of history dependence, we treat the stress-strain path as a piecewise monotone one, making use of the monotone path rule [25]. We apply an implicit time integration scheme, imposing the phase transformation conditions (3.4) and the elastic equilibrium Eq. (2.13) at selected (process) times $t_n \in [0,T]$, with $n = 1, 2, \ldots$, and $T < \infty$.

Using the notations $\mathbf{u}_n \equiv \mathbf{u}(\cdot, t_n)$, $c_n \equiv c(\cdot, t_n)$ for the displacement vector and the volume fraction at time $t = t_n$ and the symbol Δ for finite increments, we define

$$
\begin{aligned}
\Delta\mathbf{u}_n &\equiv \mathbf{u}_n - \mathbf{u}_{n-1}, \\
\Delta c_n &\equiv c_n - c_{n-1}.
\end{aligned}
$$

Further, we split the function Δc_n into its positive and negative part, cf. (3.2), obtaining the decomposition

$$\Delta c_n = \Delta c_n^+ - \Delta c_n^- .$$

Let $U(t_n)$ designate the set of kinematically admissible displacements of the body Ω at time $t = t_n$,

$$U(t_n) = \left\{ \mathbf{v} \in H^1(\Omega, \mathbb{R}^d) |\ \mathbf{v}(\mathbf{x}) = \mathbf{w}(\mathbf{x}, t_n) \text{ for a.e. } \mathbf{x} \in \partial\Omega_u \right\}$$

where $H^1(\Omega, \mathbb{R}^d)$ is a usual Hilbert space of vector-valued functions defined on Ω, i.e. the set of functions which, together with their first derivatives, are square-integrable. By $\partial\Omega_u$ we denote a part of the boundary $\partial\Omega$ where displacements $\mathbf{w}$ are prescribed (at time t_n), and let V stand for the space of test functions, defined by $V = U(t_n)$. The sets $K_+(c_{n-1})$ and $K_-(c_{n-1})$ that impose constraints on the finite, positive Δc_n^+ and negative Δc_n^- parts of increments of volume fraction take the form

$$\begin{aligned} K(z) &= \left\{ w \in L^2(\Omega) :\ 0 \le z + w \le 1,\, z \in Z \right\}, \\ K_+(z) &= \left\{ w \in L^2(\Omega) :\ w \ge 0,\, z + w \le 1,\, z \in Z \right\}, \\ K_-(z) &= \left\{ w \in L^2(\Omega) :\ w \ge 0,\, z - w \ge 0,\, z \in Z \right\}, \\ Z &= \left\{ z \in L^2(\Omega) :\ 0 \le z \le 1 \right\}, \end{aligned} \tag{3.5}$$

where $L^2(\Omega)$ is the space of square-integrable functions.

Before giving a weak formulation of the boundary value problem, we define the following bilinear and linear forms which correspond to relations (3.4) and (2.13),

$$\begin{aligned} a(\mathbf{w}, \mathbf{v}) &= \int_\Omega \mathbf{E} \nabla \mathbf{w} \cdot \nabla \mathbf{v}\, d\mathbf{x}, \\ g(w, \mathbf{v}) &= \int_\Omega w \mathbf{E} \mathbf{d} \cdot \nabla \mathbf{v}\, d\mathbf{x}, \\ h(w, v) &= \int_\Omega (\mathbf{d} \cdot \mathbf{E} \mathbf{d} + L - B) w v\, d\mathbf{x}, \end{aligned} \tag{3.6}$$

$$\begin{aligned} l_{n,n-1}(\mathbf{v}) &= \int_\Omega \Delta \mathbf{f}_n \cdot \mathbf{v}\, d\mathbf{x} + (\text{terms on } \partial\Omega)_{n,n-1}, \\ b_{n-1}^{\pm}(c_{n-1}, w) &= \int_\Omega [B/2 + (\varpi_2 - \varpi_1) + L(c_{n-1} - c_{n-1}^0)^{\pm}] w\, d\mathbf{x} \\ &\qquad \mp g(w, \mathbf{u}_{n-1}) \pm h(c_{n-1}, w). \end{aligned} \tag{3.7}$$

With these notation we can define a typical time step $t_{n-1} \Longrightarrow t_n$ of the incremental boundary value problem for the phase transformation process under consideration as the variational inequality.

$$
\text{(3.8)} \quad \boxed{
\begin{aligned}
&\text{Find} \quad (\Delta \mathbf{u}_n, \Delta c_n) \in U(t_n) \times K(c_{n-1}) \text{ such that} \\
&\qquad a(\Delta \mathbf{u}_n, \mathbf{v}) - g(\Delta c_n, \mathbf{v}) = l_{n,n-1}(\mathbf{v}) \qquad \forall\, \mathbf{v} \in V \\
&\mp g(z_\pm - \Delta c_n^\pm, \Delta \mathbf{u}_n) \pm h(\Delta c_n, z_\pm - \Delta c_n^\pm) \geq \mp b_{n-1}^\pm(c_{n-1}, z_\pm - \Delta c_n^\pm) \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall\, z_\pm \in K_\pm(c_{n-1})
\end{aligned}
}
$$

Having solved (3.8) for increments $\Delta \mathbf{u}_n$ and Δc_n, we can easily update the discrete memory c_{n-1}^0 to c_n^0 at the current time $t = t_n$, details are given in [25].

Under the usual assumptions including those of symmetry and pointwise stability of the elasticity tensor $\mathbf{E}$, and provided that the set $\partial \Omega_u$ has a positive measure and excludes rigid motions of the body Ω, the following result can be proved, [21].

THEOREM 3.2. *Let the material parameters $L, B \geq 0$ satisfy the inequality $L \geq B$. Then the problem (3.8) possesses a solution. The solution is unique, provided $L > B$.*

The first equation of the system (3.8) is a weak form of the equilibrium conditions (2.13), whilst $(3.8)_2$ represents two variational inequalities which are a weak form of the phase transformation rules (2.11) in virtue of the equivalence lemma (3.1) and expressions (3.4). The system (3.8) can conveniently be discretized in space by the finite element method and is solved finally as a standard form of the linear complementarity problem, after some rearrangements due to the restricted variations of the variables Δc_n^+, Δc_n^- and the fact that changes $\Delta \mathbf{u}_n$ of the displacement vector are not restricted in sign.

3.3. Linear complementarity problem

Let $\varphi_i(x)\,(1 \leq i \leq N)$ and $\psi_j(x)\,(1 \leq j \leq M)$ be the finite element bases we use for the displacement $\mathbf{u}$ and phase fraction c in $H^1(\Omega)$ and $L^2(\Omega)$. In particular, the field of displacement $\mathbf{u}$ can be approximated by a piecewise quadratic polynomial, whereas for the function of phase fraction c (and c^0) a piecewise linear approximation can be utilized. We remark that using of piecewise linear basis functions ψ_j leads to the internal approximation of the sets $K_\pm$ in (3.5).

The finite-dimensional counterpart of the weak formulation (3.8) may be expressed as the following linear complementarity problem:

$$\boxed{\begin{gathered}\mathbf{D}\mathbf{x}_n + \mathbf{y}_n = \mathbf{b}_{n,n-1}\\ \mathbf{x}'_n \geq \mathbf{0},\ \mathbf{y}^1_n = \mathbf{0},\ \mathbf{y}_n \geq \mathbf{0},\ \mathbf{x}_n{\cdot}\mathbf{y}_n = 0\end{gathered}} \tag{3.9}$$

in which $\mathbf{D}$ is a square matrix, $\mathbf{x}_n$ is a vector of unknowns (nodal values of the finite element approximations), $\mathbf{y}_n$ denotes a vector of slack variables, and the vector $\mathbf{b}_{n,n-1}$ is known at time t_n. By $\mathbf{x}'_n$ we denote the elements of the vector $\mathbf{x}_n$, excluding the subvector $\mathbf{x}^1_n \equiv \Delta\mathbf{u}_n$ which is sign-unrestricted. The above matrix and vectors have the following structure:

$$\mathbf{D} = \begin{bmatrix} -\mathbf{K} & \mathbf{G}^{\mathrm{T}} & -\mathbf{G}^{\mathrm{T}} & \mathbf{0} & \mathbf{0}\\ \mathbf{G} & -\mathbf{H} & \mathbf{H} & -\mathbf{I} & \mathbf{0}\\ -\mathbf{G} & \mathbf{H} & -\mathbf{H} & \mathbf{0} & -\mathbf{I}\\ \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \mathbf{I} & \mathbf{0} & \mathbf{0}\end{bmatrix}, \quad \mathbf{x}_n = \begin{Bmatrix} \Delta\mathbf{u}_n\\ \Delta\mathbf{c}^+_n\\ \Delta\mathbf{c}^-_n\\ \mathbf{r}^1_n\\ \mathbf{r}^0_n\end{Bmatrix},$$

$$\mathbf{b}_{n,n-1} = \begin{Bmatrix} \mathbf{b}^u_{n,n-1}\\ \mathbf{b}^{c^+}_{n-1}\\ \mathbf{b}^{c^-}_{n-1}\\ \mathbf{1}-\mathbf{c}_{n-1}\\ \mathbf{c}_{n-1}\end{Bmatrix}.$$

Matrices $\mathbf{K}, \mathbf{G}$ and $\mathbf{H}$ are generated by the bilinear forms (3.6),

$$\begin{aligned}\mathbf{K} &= [K_{ij}] = [a(\varphi_i,\varphi_j)], \quad \dim\mathbf{K} = N\times N,\\ \mathbf{G} &= [G_{ij}] = [g(\psi_i,\varphi_j)], \quad \dim\mathbf{G} = M\times N,\\ \mathbf{H} &= [H_{ij}] = [h(\psi_i,\psi_j)], \quad \dim\mathbf{H} = M\times M,\end{aligned}$$

and $\mathbf{I}$ is the $M\times M$ identity matrix corresponding to the vectors $\Delta\mathbf{c}^+_n$, $\Delta\mathbf{c}^-_n$ and their conjugates $\mathbf{r}^1_n$, $\mathbf{r}^0_n$. The latter are Lagrange's multipliers which are induced by the constraint imposed on the volume fraction that $c \in [0, 1]$, cf. footnote 1 in LEMMA 3.1. Vectors $\mathbf{b}^u_{n,n-1}$, $\mathbf{b}^{c^+}_{n-1}$ and $\mathbf{b}^{c^-}_{n-1}$ are generated by the linear forms (3.7). The matrices $\mathbf{K}$ (stiffness matrix) and $\mathbf{H}$ are symmetric and positive definite. For the solution of problem (3.9) we developed our own computer program based on the algorithm presented in [22].

4. Numerical results

Our goal here is to check numerically the presented formulation and to see the consequences of the assumptions taken. We have simulated the basic, uniaxial tension test on a strip made from a two-phase material, as a plane stress displacement-driven problem. The strip and the imposed boundary conditions (4.1) are schematically displayed in Fig. 3. In the coordinate axis xy, let the displacement vector $\mathbf{u} = (u, v)$ have the components u and v, and let the length and width of the strip be a and b, respectively. We assumed the following boundary conditions:

$$
(4.1)\qquad
\begin{aligned}
&\text{on the left-hand side of the strip} && \begin{cases} u(0,y) = 0 & 0 \le y \le b, \\ v(0,b/2) = 0, \end{cases} \\
&\text{on the right-hand side of the strip} && \begin{cases} u(a,y) = w(t) & 0 \le y \le b, \\ v(a,b/2) = 0. \end{cases}
\end{aligned}
$$

The loading program $w(t)$ is a bilinear hat function, increasing from zero to the scaled maximum value of $w(t')/a = 0.050833$ at a time $t = t'$, and then decreasing to zero.

For the field of displacements $\mathbf{u}(\cdot,t) \equiv (u(\cdot,t), v(\cdot,t))$ we have used a 6-node triangle finite element with quadratic shape functions (linear strain triangle), whilst for the volume fraction $c(\cdot,t)$ a 3-node linear triangle. The uniform mesh of $(6\times18)\times4$ finite elements we employed is shown in Fig. 3. Due to the difficulty

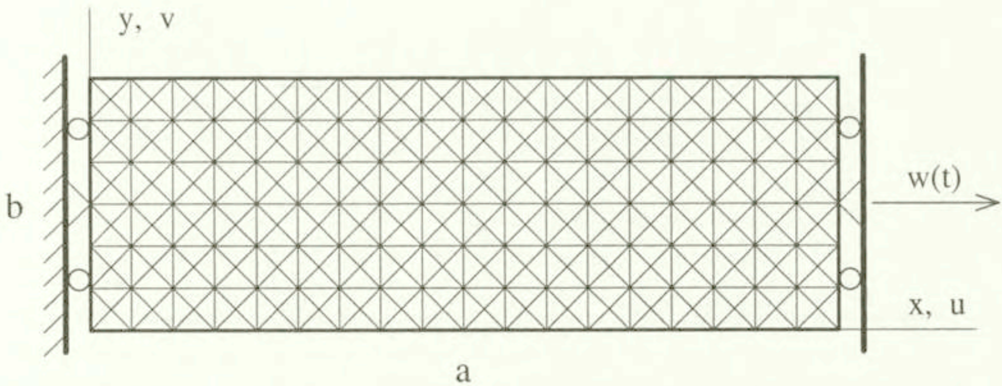
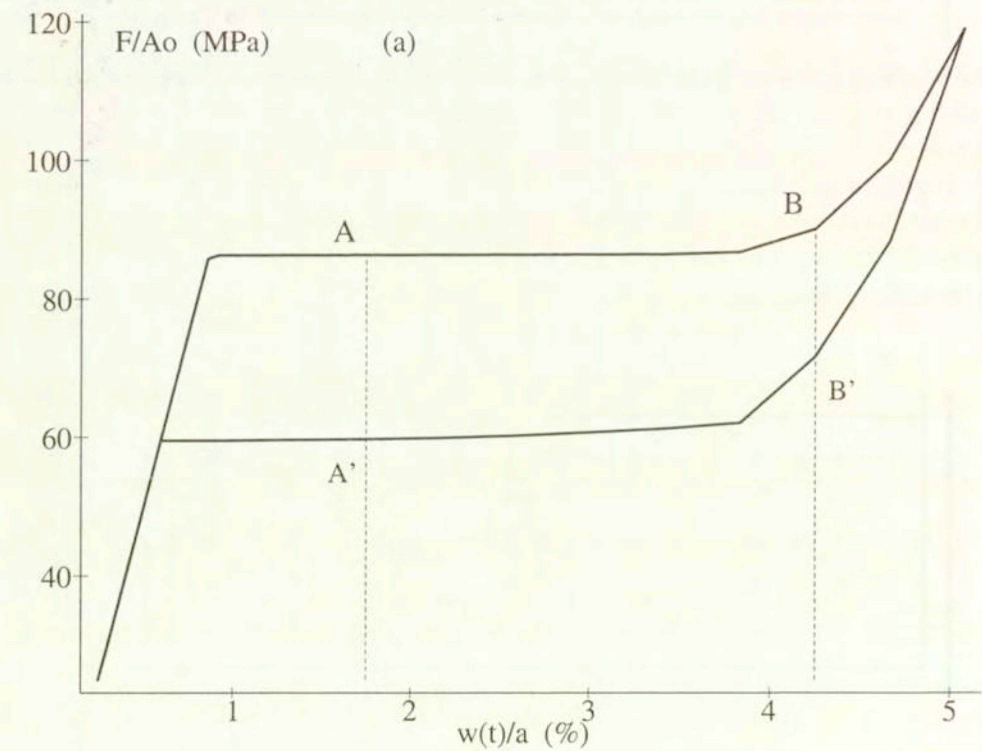


FIG. 3. The strip made of a material with two preferred states, of length a and width b with $a : b = 12 : 4$, under uniaxial tension $w(t)$.

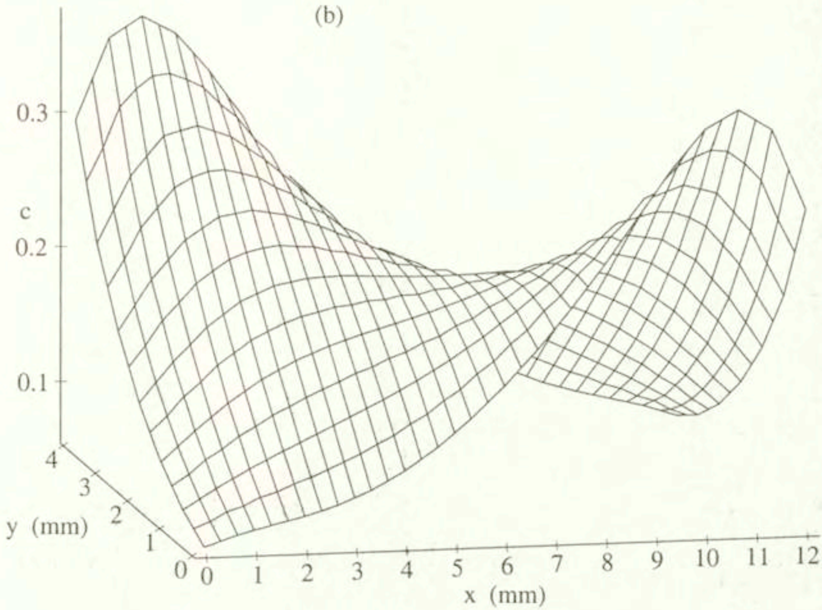
in finding all the needed parameters for a specific material, we have assumed the following material parameters corresponding to a CuZnAl single crystal [16]: $E = 10000.00$ MPa, $B = 1.20$ J/m^3, $L = 1.01B$, $\nu = 0.30$, $\varpi_2 - \varpi_1 = 3.756$ J/m^3, the thresholds $\kappa_{1\to 2}$ and $\kappa_{2\to 1}$ by (2.9), and the transformation strain corresponding to one variant of a CuAlNi alloy [5],

$$\mathbf{d} = \begin{bmatrix} 0.045 & 0.020 \\ 0.020 & 0.045 \end{bmatrix}.$$

Using the same material data, we have calculated the strip for two proportions of its length to width: case 1 with $a : b = 12$ mm : 4 mm, and case 2 with $a : b = 24$ mm : 4 mm, and the same thickness of 0.4 mm. In its initial state the strip was in the austenite phase, and $c(\mathbf{x}, t_0) = c^0(\mathbf{x}, t_0) = 0$, $\mathbf{x} \in \Omega = [0, a] \times [0, b]$. The characteristic major hysteresis loop is shown in Fig. 4a. Displayed is the relation between the force F at the side ($x = a, 0 \le y \le b$), divided by the initial cross-sectional area A_0 of the strip, versus the scaled elongation $w(t)/a$. On the graph two pairs (A,A') and (B,B') of states corresponding to the same scaled elongation but with different histories are marked. Figs. 4b and c, and Fig. 6



[Fig. 4a]



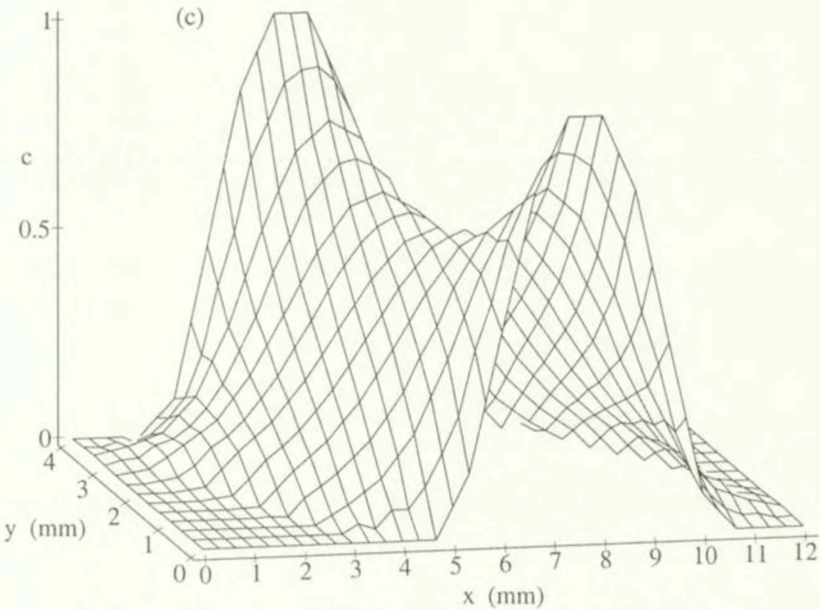
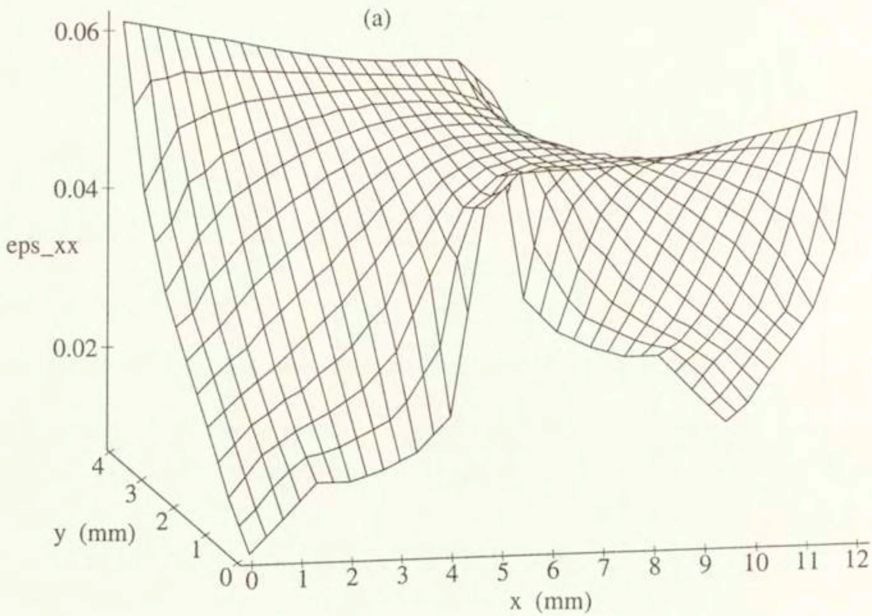
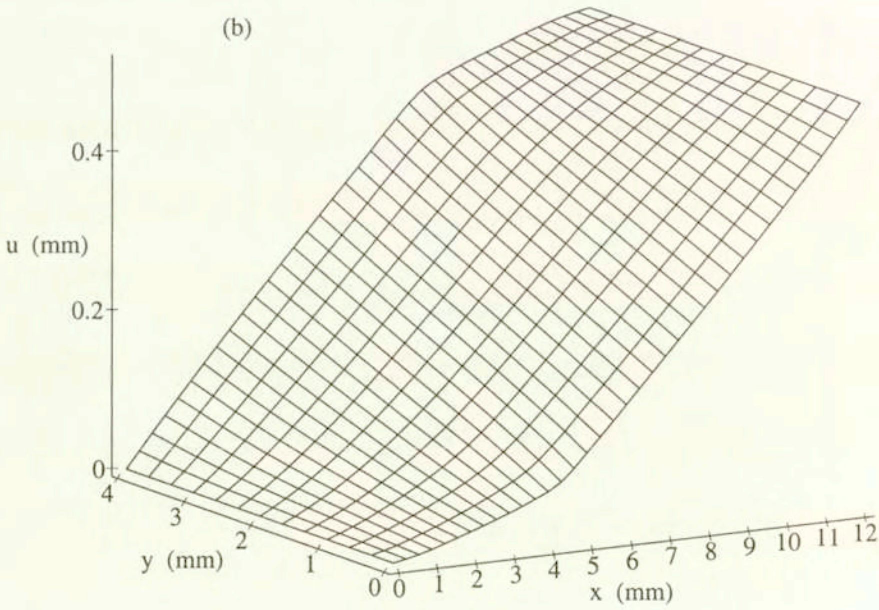


FIG. 4. Case 1. The 12×4 strip under uniaxial extension program $w(t)$. (a) Major hysteresis loop in the scaled force—elongation space (F/A_0) — $(w(t)/a)$, (b) and (c) Distribution of c at the corresponding states A and A$'$.


(a)
0.06
0.04
eps_xx
0.02
4
3
2
1
0
y (mm)
0 1 2 3 4 5 6 7 8 9 10 11 12
x (mm)


(b)
0.4
u (mm)
0.2
0
4
3
2
1
0
y (mm)
0 1 2 3 4 5 6 7 8 9 10 11 12
x (mm)

[Fig. 5a, b]

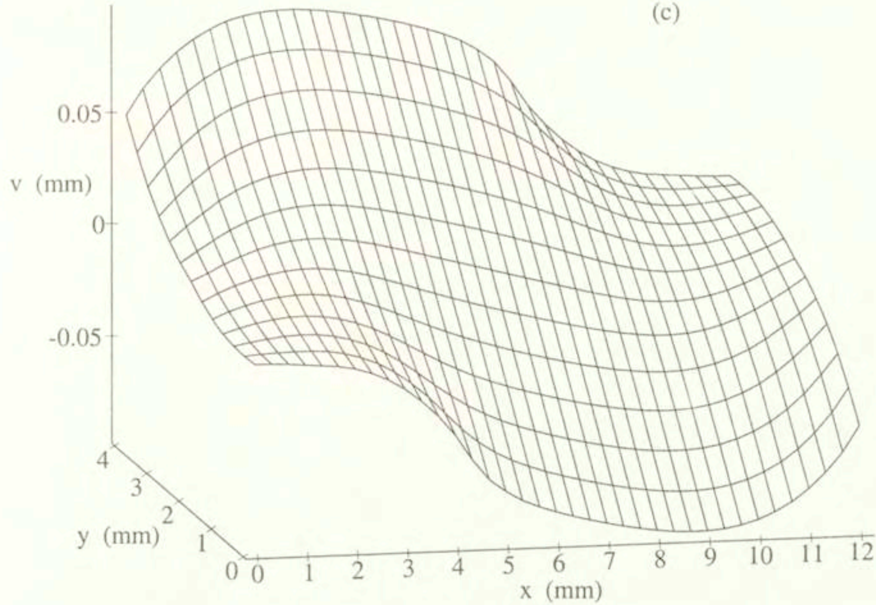


FIG. 5. Case 1. Distributions of strain ϵ_{xx}, (a), and the corresponding displacement u along the elongation, (b), and perpendicular displacement v, (c), at the state B in Fig. 4.

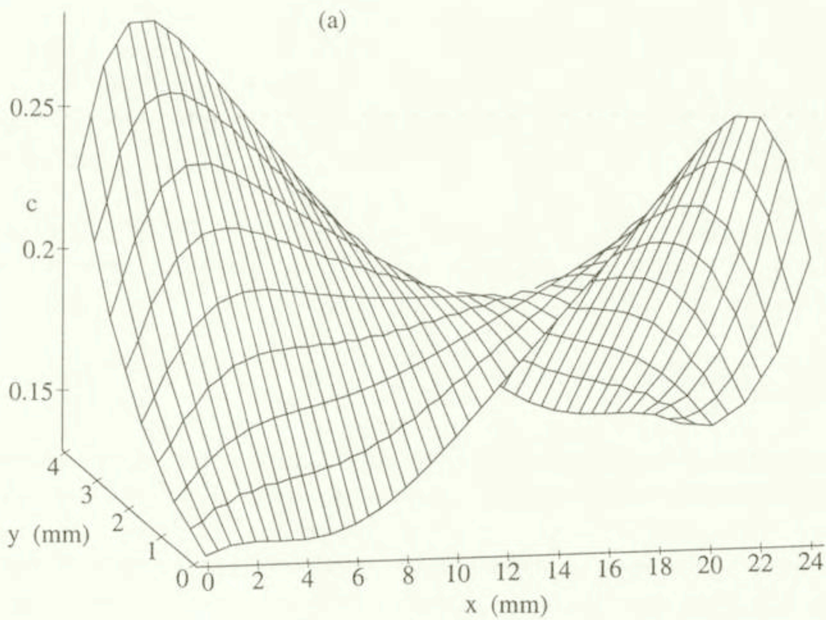


FIG. 6a]

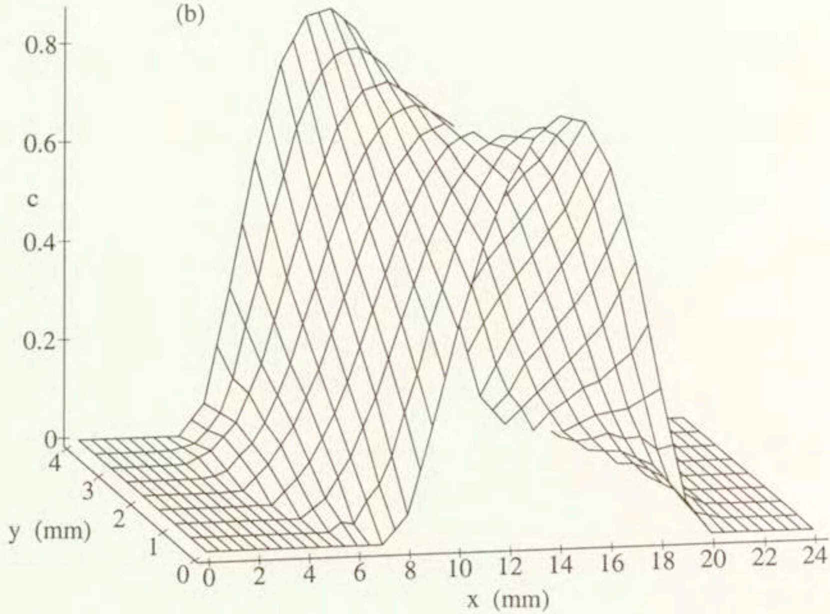


FIG. 6. Case 2. The 24×4 strip under uniaxial extension program $w(t)$. (a) and (b) Distribution of c at the states corresponding to A and A′ in Fig. 4.

reveal that the extension of the two-phase strip induces inhomogeneous fields whose paths of evolution do not coincide during the loading and unloading stages, even for this simple uniaxial loading program. Observe also that the initially straight axis ($0 \leq x \leq a, y = b/2$) of the strip does not remain straight in the xy-plane in the course of the process, see Fig. 5c for the component v of the displacement vector $\mathbf{u}$. Finally, it is worthy to mention that the proposed formulation allows us to determine the solution of this initially homogeneous problem without introducing any disturbance to the system in order to initiate the phase transformation.

5. Closing remarks

In the paper, a variational inequality approach to the hysteresis behaviour of a two-phase system undergoing thermoelastic martensitic transformations is developed. The starting point is a homogenized free energy for the mixture of two phases, in the setting of linearized theory of elasticity with a parabolic energy function for each phase. The mathematical model proposed is a weak expression of the equilibrium conditions and the phase transformation rules. The latter take into account the characteristic dissipative effects of friction type and comply with the second principle of thermodynamics; they constitute an implicit form of the equation of kinetics of the phase transformation. To solve the rate variational inequality, a computational algorithm is devised which comprises an implicit time integration scheme and a mathematical programming procedure (linear complementarity problem). The existence of a unique solution to the problem considered is assured. The numerical results obtained for the tension test on austenite-martensite strips show that, even in the two-phase system, two corresponding states on the force-elongation diagram are connected with different inhomogeneous states in the bulk of the sample. In future work we will concentrate on the case of multi-phase systems. Also, accounting for the effects of plasticity and temperature is desirable.

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